### Final Technical Report

for

# Computation of Reacting Flows in Combustion Processes

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## COMPUTATION OF REACTING FLOWS IN COMBUSTION PROCESS WITH UNSTRUCTURED GRIDS

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#### **ABSTRACT**

The objective of this research is to develop an efficient numerical algorithm with unstructured grids for the computation of three-dimensional chemical reacting flows that are known to occur in combustion components of propulsions systems. During the grant period (1996 to 1999), two companion codes have been developed and various numerical and physical models were implemented into the two codes.

#### **SUMMARY**

Research activities during this grant period were focused on (1) improving the code capabilities of the CORSAIR and (2) developing an alternative flow solver, FLUX, using a new space-time algorithm. The individual research activities are summarized as follows.

#### (1) CORSAIR:

COSRAIR is a general unstructured three-dimensional combustion CFD code. It employs fourth-order Runge-Kutta time integration scheme. The code is also equipped with a time pre-conditioning technique to efficiently handle low Mach number compressible flows. The mixed volume grid approach used in the code greatly enhances the gridding capability that can place a most suitable type of mesh in any part of the flow domain. The various types of mesh are then combined to describe the entire geometry. The code is highly parallelized using automatic domain decomposition that can be run on various workstation platforms and multi-processors. It comes with a standard turbulence model and uses a wall function for turbulent flow modeling at flow boundaries. The enhancements for the code are:

- 1. Implementation of a low-Reynolds turbulence model to ease some of the insistency of using the original wall function in the code.
- 2. Implementation of a new non-linear turbulence model with a wall distance model to better predict turbulent swirling flows.
- 3. Implementation of a new non-linear turbulence model without wall distance information to eliminate the lengthy calculation of wall distance in complex three-dimensional geometries with many wall boundaries.
- 4. Implementation of an implicit physical time numerical treatment to greatly improve the stability range of the pseudo-time stepping for low speed transient calculations.
- 5. Implementation of a generalized chemistry formulation that allows users to easily specify the species of reacting flows. With this capability, any, user-defined, chemistry kinetics can be applied directly from the input files without the necessity of having to change the code.

6. Compilation of a suite of test cases for benchmark testing of the National Combustion Code (NCC) beta release, version 1.0. The purpose of this effort is to provide a standard suite of test cases that are documented with detailed computer time usage, number of processors (or workstations), running environment and numerical performance in terms of convergence and solution accuracy for the users and code developers.

#### (2) FLUX

The FLUX code uses a newly developed space-time numerical algorithm. The new algorithm utilizes the same mesh structure and thus can share the grid and result data files with CORSAIR. The strength of the FLUX algorithm is that it may be used for high-speed unsteady computation and possesses a high-quality shock capturing capability. Both two and three-dimensional, inviscid and viscous flow capabilities were implemented in the code. The activities for the FLUX code development are:

- 1. Development of the first true unstructured mesh code using the space-time numerical algorithm and extension of the unstructured algorithm to three-dimensional flow calculations.
- 2. Demonstration of various low and high-speed flow calculations for both inviscid and viscous flows.
- 3. Publication of two papers that document the above developments.

#### RESEARCH PUBLICATIONS

The following is a list of publications produced during the grant period.

- 1. Chen, K.-H. and Liu, N.-S., "Navier-Stokes Solution of the FLUX Code: A Module for the NCC solver Using the Concept of Space-Time Conservation Element and Solution Element," presented at the 38<sup>th</sup> Aerospace Sciences Meeting and Exhibit, January 10-13, 2000/Reno, NV, AIAA 2000-0455.
- 2. Shih, T.-H., Povinelli, L. A., N.-S. Liu, and Chen, K-H., "Generalized Wall Function for Complex Turbulent Flows," presented at the 38<sup>th</sup> Aerospace Sciences Meeting and Exhibit, January 10-13, 2000/Reno, NV, AIAA 2000-0332.
- 3. Liu, N.-S. and Chen, K.-H., "FLUX: An Alternative Solver for the National Combustion Code," presented at the 37th AIAA Aerospace Sciences Meeting and Exhibit, January 11-14, 1999/Reno, NV, AIAA 99-1079.
- 4. Chen, K.H., Norris, A., Quealy, A., and Liu, N.S., "Benchmark Test Cases for the National Combustion Code," presented at the 34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, July 13-15, 1998/Cleveland, OH, AIAA 98-3855.
- 5. Shih, T.H., Chen, K.H., and Liu, N.S., "A Non-linear k-e Model for Turbulent Shear Flows," presented at the 34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, July 13-15, 1998/Cleveland, OH, AIAA 98-3983.

- 6. Chen, K.H. and Liu, N.S., "Evaluation of a Non-Linear Turbulence Model Using Mixed Volume Unstructured Grids," presented at the 36th AIAA Aerospace Sciences Meeting and Exhibit, January 12-15, 1998/Reno, NV, AIAA 98-0233.
- 7. Shih, T.H., Zhu J., Liou, W., Chen, K.H., Liu, N.-S., and Lumley, J. L., "Modeling of Turbulent Swirling Flows," NASA TM 113112, Aug. 1997.
- 8. Chen, K.H. and Friker, D., "Parallelization of Lagrangian Spray Combustion by Domain Decomposition," 9th Annual Symposium, pp. 101-106, Propulsion Engineering Research Center, Penn State University, Oct. 1-2, 1997.
- 9. Shih, T.H., Zhu J., Liou, W., Chen, K.H., Liu, N.-S., and Lumley, J. L. "Modeling of Turbulent swirling Flows," *Proceedings of the 11<sup>th</sup> symposium on Turbulent Shear Flows*, Grenoble, France, Sep. 8-11, 1997.
- 10. Chen, K.H. and Keith, T., "Numerical Study of Three-Dimensional Air Flow Characteristics in a Throttle Body with Chimera Grid," Conference Proceedings, pp. 487-492, 2nd Asian Computational Fluid Dynamics Conference, Tokyo, Japan, 15-18, 3/4/013/4/01Dec. 1996.
- 11. Chen, K.H., DelSignore, D. and Keith, T., "Numerical and Experimental Study of Three-Dimensional Air Flow Characteristics in a Throttle Body," Conference Proceedings, pp. 439-448, International Congress on Fluid Dynamics and Propulsion, Cairo, Egypt, 29-31, Dec. 1996.
- 12. Chen, K.H. and Bulzan B., "Numerical Study of Cooling System Design in a High Pressure combustion Rig with Chimera Grids," presented at the 32nd AIAA/ASME/SAE/ASEE Joint Propulsion conference and Exhibit, July 1-3, 1996/Lake Buena Vista, FL, AIAA 96-3126.
- 13. Yungster, S. and Chen, K.H., "Application of Chimera Grid Scheme to Combustor Flow fields at all Speeds," presented at the 34th AIAA Aerospace Sciences Meeting and Exhibit, January 15-18, 1996/Reno, NV, AIAA 96-0731.